Jmol, a java molecular viewer

Fabian Dortu

Jmol history

- Jmol was started in 2000 by Dan Gezelter (OpenScience project's director) as a replacement to XMol.
- Jmol is an OpenScience project.
- Jmol is under the terms of the GNU Lesser General Public License (LGPL).

Project history and participant

- Project leader
  - Dan Gezelter (OpenScience project's director)
  - Bradley Smith
  - Egon Willighagen (Actual project leader)
- Project members
  - Egon Willighagen
  - Fabian Dortu
  - Dan Gezelter
  - Michael T. Howard
- Many contributors who joined the project by sending patches to make Jmol fit their own needs

Features Overview

- Support many type of files:
  - ***ABINIT***
  - ACES II
  - ADF
  - CML (Chemical Markup Language) E. Willighagen
  - Dalton
  - GAMESS
  - Gaussian 90/92/94/96/98
  - Ghemical
  - Jaguar
  - MDL Molfile
  - MOPAC 7/97/2002
  - PDB
  - XYZ

Features overview

- 3D representation of molecules and crystals
  - Fast pseudo 3D rendering
  - high quality output with povray rendering
  - **java3D / GL4Java rendering**
- Animates the result of simulations
- Display measurements inter-atomic distances, bond angles and dihedral angles from atomic coordinates as a simulation progresses.

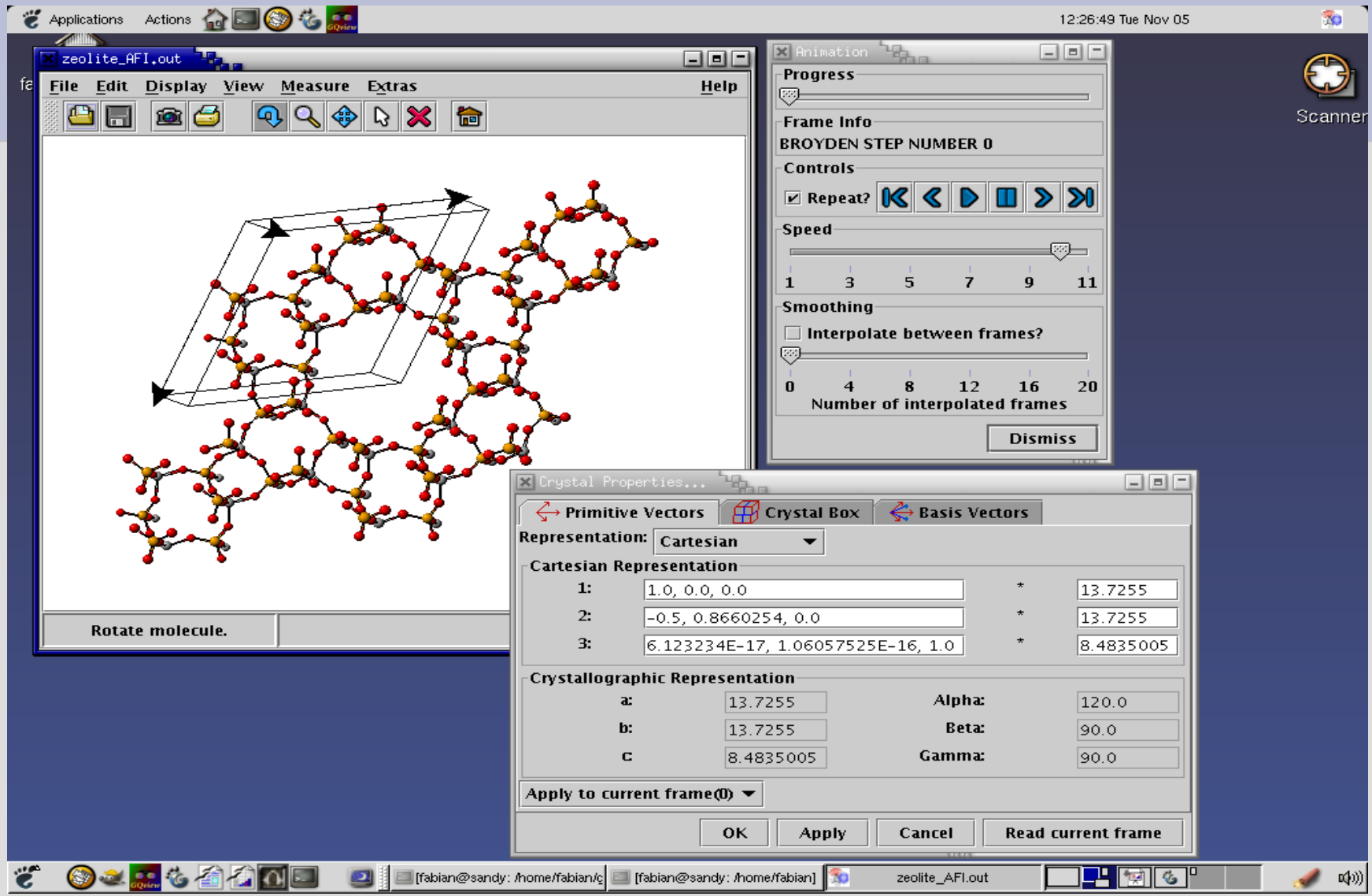
Features Overview

- Animates the computed vibration modes (not yet available for ABINIT).
- Display vectors (velocity, dipole, etc), charges, atomic symbols or atomic indexes during animation.
- Exports frames as images
  - gif, jpg, ppm, bmp, png,pdf
- Representation of graphable properties
  - energy vs. step number
  - **band diagrams**
  - **phonon dispersion curves**
- Java applet

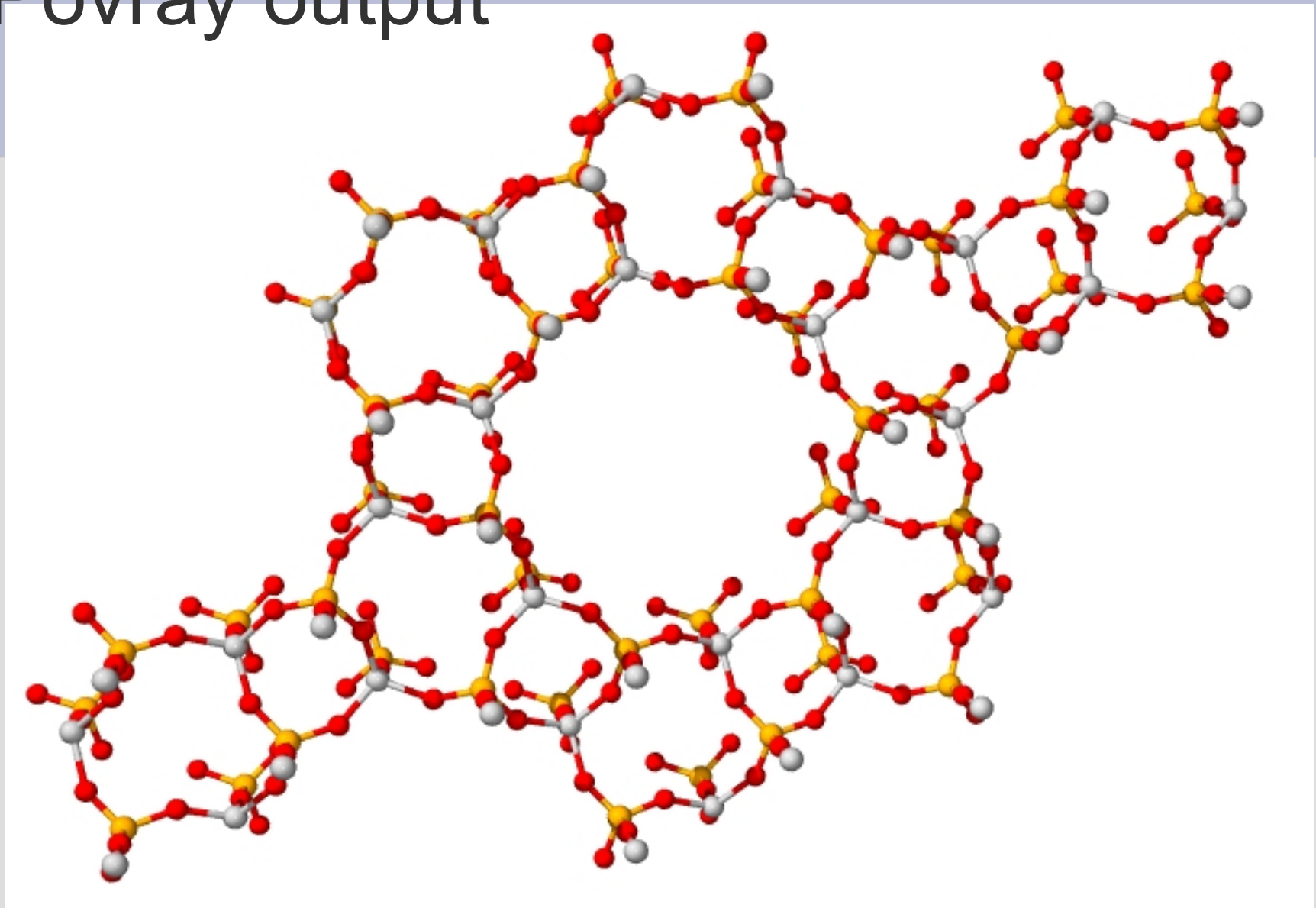
Abinit Features

- Abinit *input* files
  - multi dataset *not* supported.
- Abinit *output* files
  - muli dataset support
  - multi frame support(molecular dynamics, optimization)
  - reading of frame energy
  - **reading/plotting of band diagram (soon)**
  - **reading/plotting of phonon dispersion curve and mode animation.**

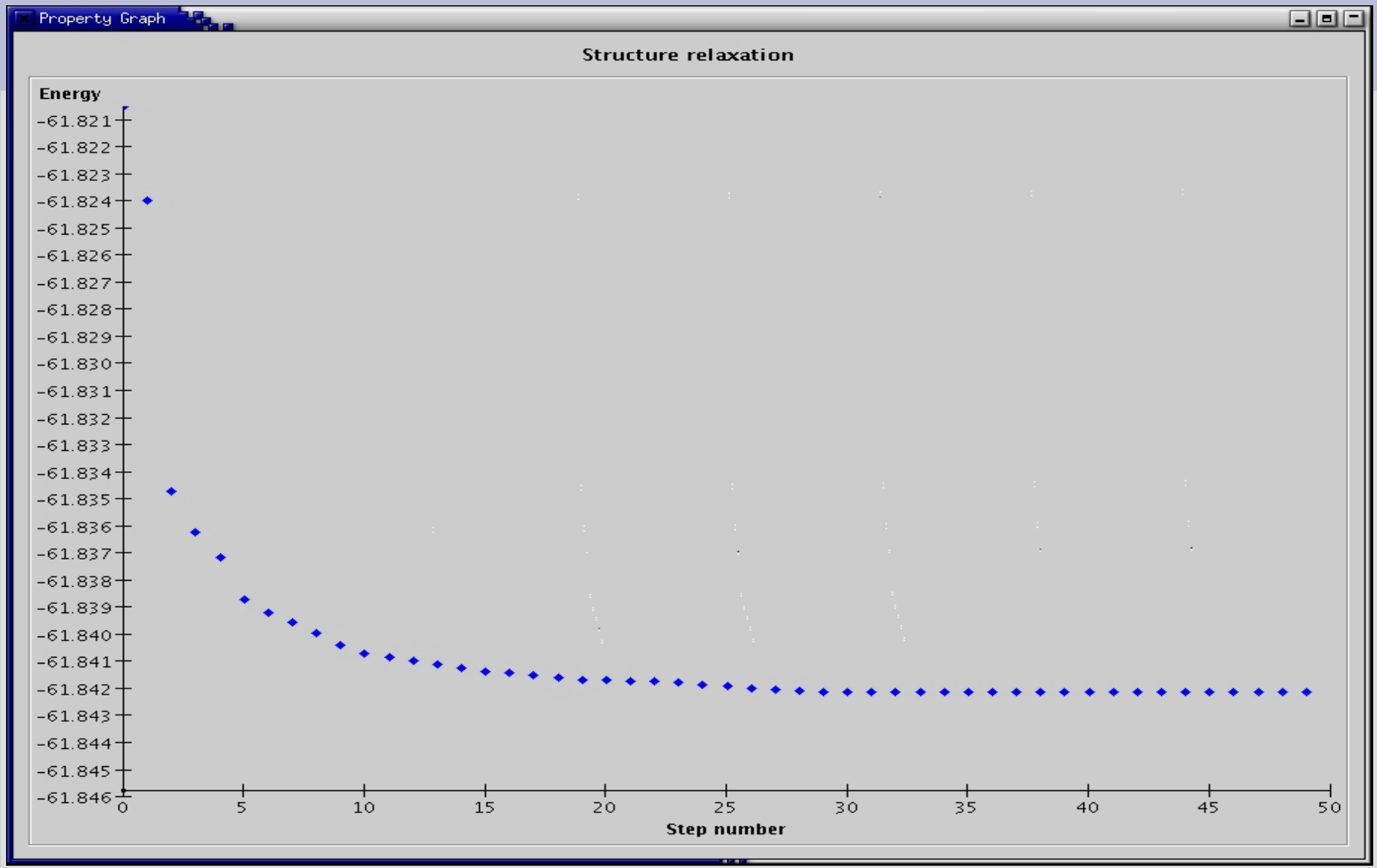
Snapshot


Applications
Actions
12:26:49 Tue Nov 05
zeolite_AFI.out
File Edit Display View Measure Extras Help
Rotate molecule.
Animation
Progress
Frame Info
BROYDEN STEP NUMBER 0
Controls
Repeat?
Speed
1 3 5 7 9 11
Smoothing
Interpolate between frames?
0 4 8 12 16 20
Number of interpolated frames
Dismiss
Crystal Properties...
Primitive Vectors
Crystal Box
Basis Vectors
Representation: Cartesian
Cartesian Representation
1: 1.0, 0.0, 0.0 * 13.7255
2: -0.5, 0.8660254, 0.0 * 13.7255
3: 6.123234E-17, 1.06057525E-16, 1.0 * 8.4835005
Crystallographic Representation
a: 13.7255
b: 13.7255
c 8.4835005
Alpha: 120.0
Beta: 90.0
Gamma: 90.0
Apply to current frame(0)
OK
Apply
Cancel
Read current frame
Scanner
[fabian@sandy: /home/fabian/c
[fabian@sandy: /home/fabian]
zeolite_AFI.out

Povray output

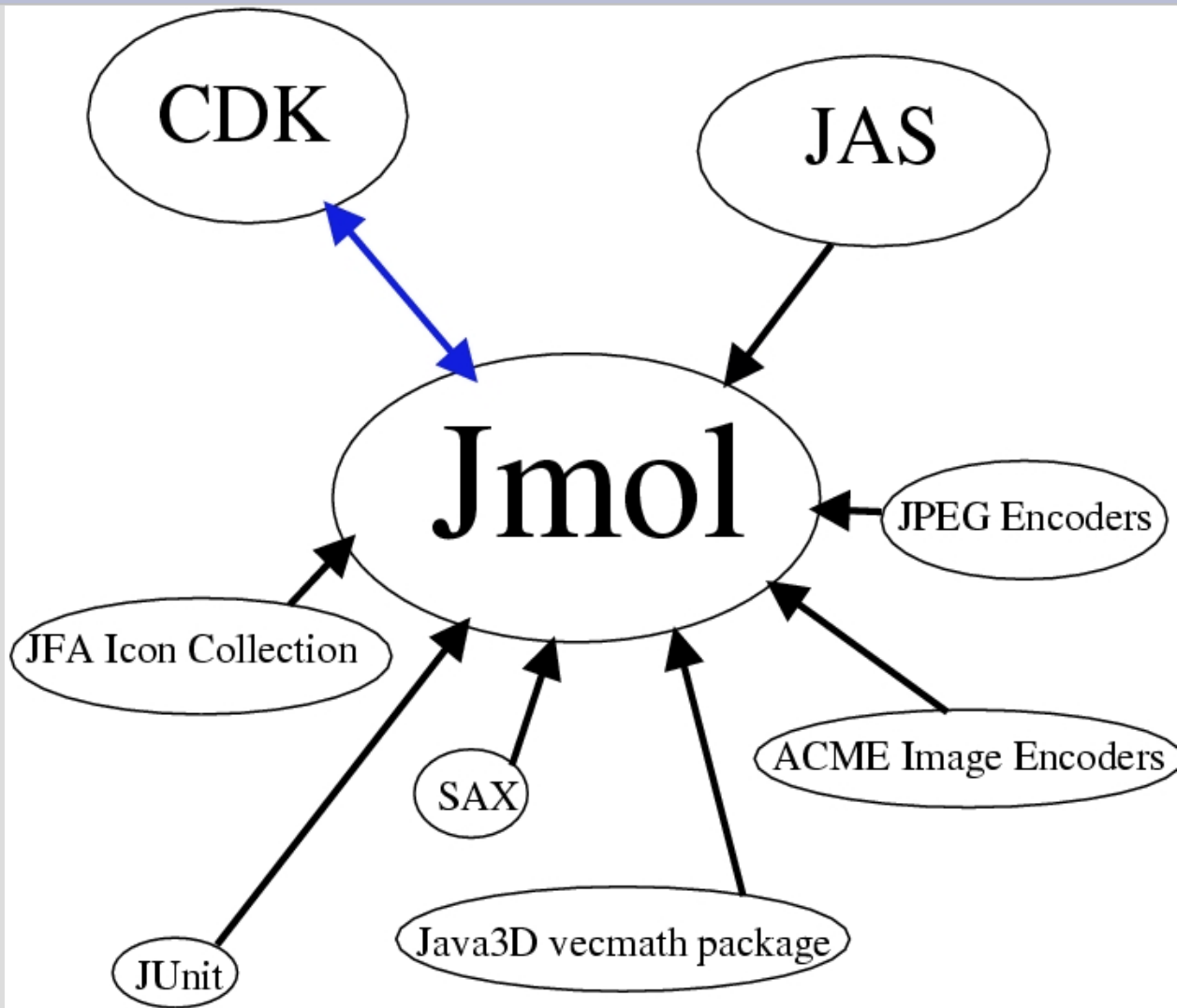


Graphs


Property Graph
Structure relaxation
Energy
-61.821
-61.822
-61.823
-61.824
-61.825
-61.826
-61.827
-61.828
-61.829
-61.830
-61.831
-61.832
-61.833
-61.834
-61.835
-61.836
-61.837
-61.838
-61.839
-61.840
-61.841
-61.842
-61.843
-61.844
-61.845
-61.846
0
5
10
15
20
25
30
35
40
45
50
Step number

Noteworthy libraries

- **Chemical Development Kit (CDK) : Java utility classes for ChemoInformatics and Computational Chemistry by Egon Willighagen.**
- **Java Analysis Studio (JAS) : Java utility classes for data representation.**



Goals for the future

- *Main goal:* Port Jmol to the CDK.
  - code factorization/modularization
  - CDK provides standard containers for chemical entities like atoms and bands.
  - algorithm used in Jmol are of general interest outside Jmol and will be ported to CDK.
  - the merge of Jmol and CDK community focuses the open source effort and would have benefits for both community

Goals for the future

- *Goal 2*: add functionalities to the Jmol applet
- *Goal 3*: better documentation
  - developer's guide: describe the architecture and algorithms used in Jmol.
  - JavaDocs: understand how classes are structured.
  - user's guide: features and uses of Jmol.
- *Goal 4*: Implementing more features while keeping the code stable and working on modularization
  - will move to a 2 branches development model

Goals for the futures

- *Goal 5: Getting in touch with the Jmol user base*
  - *who is using Jmol ?*
  - *what are user's wishes ?*

  We need feedback!!!
  - *tell us what features you would have!*
  - *send me ABINIT sample files!*

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The OpenScience Project

What is the OpenScience Project?

- The OpenScience project is dedicated to writing and releasing Open Source scientific software.
- We are a group of scientists, mathematicians and engineers who see the scientific benefit of the peer review that open source software provides.
- We want to encourage a collaborative environment in which science can be pursued by anyone who is inspired to discover something new about the natural world.